Directly revealing charge-induced molecular dissociation and the reactivity of the reconstructed structure at the atomic scale

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Catalytic activity plays a pivotal role in chemical transformations, where creating abundant active sites through nanostructuring strategies enhances surface area and exposes reactive crystallographic facets. Here, we directly revealed the geometric structure and surface potential of (1×2) reconstruction on rutile TiO_2(110) with atomic resolution using non-contact atomic force microscopy and Kelvin probe force microscopy. As a result, the charge accumulation of the (1×2) reconstruction on the surface can be clearly observed, indicating the higher reactivity of this reconstructed surface for catalysis. We found that the reconstruction process facilitates easier oxygen molecule dissociation due to its higher surface potential. This higher potential is influenced by excess electrons, which are induced by polaron. This finding is corroborated by density functional theory calculations. Directly measuring the characteristics of reconstruction with atomic resolution can provide a more profound understanding of surface reactivity. Moreover, this research sheds light on the surface reconstructing, phase transitions, and defect engineering.

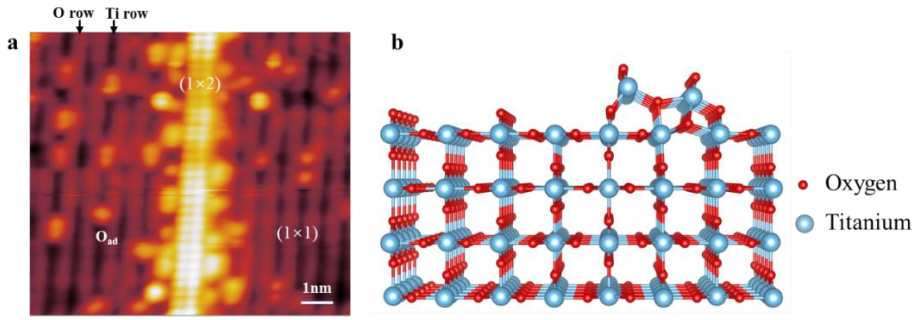

Figure 1. Atomically resolved AFM image of (1×2) reconstruction on oxidized rutile TiO_2(110) surface. a Constant Δf topographic image. **b** Perspective view of ball model of rutile TiO_2(110) surface with (1×1) structure and (1×2) reconstruction. Oxygen rows: bright rows; titanium rows: dark rows. The (1×2) reconstruction: brighter rows. O_{ad}: oxygen adatom (bright spot). Scanning parameter: f_0 = 1.12 MHz, A = 500 pm, Q = 14360. Size: 10×10 nm^2.

Reference

[1] Z. Zhang, et al. Phys. Rev. Lett., **99** 126105 (2007).

[2] Q. Z. Zhang, et al. J. Am. Chem. Soc., **140** 15668-15674 (2018).